Intellectual information technologies for the study of filtration in multidimensional nanoporous particles media

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Abstract

High-performance intellectual information technologies for the nanoporous filtration systems research based on the mathematical model of the two-level transport "filtrationconsolidation" in the system of nanopores in intraparticle spaces, which includes two subspaces of particles of different sizes has been considered.

The high-speed analytical solution of the model, which allows calculations parallelization on multi-core computers has been found using the operational Heaviside's method, Laplace integral, and Fourier integral transformations.

The high-performance software complex was built on top of the mode, with a modern approach to software design and keeping in mind software engineering best practices. Numerical modeling of filtration kinetics process research has been done using developed software.

Keywords¹

Filtration processes, numerical modeling, parallel computing, science-intensive technologies, multidimensional nanoporous particles media

1. Introduction

Complex systems and processes design in the field of environmental protection, emission reduction, medicine, liquids or gases filtration requires a new high-performance information systems creation for their research based on scientific mathematical models with high-quality physical substantiation of the composition of their elements, connections between them and parameters that determine efficiency their progress and work.

The proposed information research technology of nanoporous filtration systems is based on the phenomenological model of a solid-liquid liquid that we developed, containing various-sized nanoporous moisture-containing particles as a multi-level porous system with interparticle and intraparticle networks for fluid express flows. Mathematical models of the two-level transport "filtration-consolidation" in the system "interparticle space - nanoporous particles" are considered, which take into account the internal flow of liquid from particles, along with the flow of liquid in the skeleton [1, 2].

We consider the nanoporous particles containing liquid as a porous layer subjected to unidimensional pressing (Fig. 1). The liquid flowing occurs inside the particles, outside the nanoporous particles and between these two spaces. The nanoporous particles are separated by the porous network. The layer of particles is considered a double-porosity media. Fig. 1 illustrates two levels of the considered elementary volume: level 1(a) for the system of macropores in interparticle

ITTAP'2022: 2nd International Workshop on Information Technologies: Theoretical and Applied Problems, November 22-24, 2022, Ternopil, Ukraine

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spaces and level 2 (b and c) for the system of nanopores in intraparticle spaces, which includes two subspaces of particles of different sizes: intraparticle spaces 1 - subspace of nanoporous particles with a radius of at least R₁ and intraparticle spaces 2 - a subspace of nanoporous particles with a radius of at least R₂ (R₁> R₂). The model assumed, that in nanoporous media, the first porosity level is formed by the interparticle network with low storage capacity, while two-second levels of porosities are formed by the intraparticle network with high storage capacity.

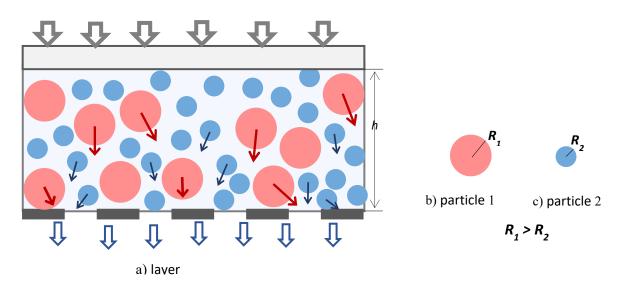


Figure 1: Example figure Schematization of mass transfer in a two-level system of pores

2. Mathematical model

The mathematical model of the considered transfer, taking into account the specified physical factors, can be described in the form of such a system of boundary value problems for equations in partial derivatives, formulated both for the interparticle space and for two intraparticle networks versus the pressure in the liquid phase.:

2.1. Consolidation equation for a layer

Problem A is to find a limited solution of the consolidation equation for a layer of multidimensional nanoporous particles media in the domain $D_1 = \{(t,z): t > 0, 0 < z < h\}$:

$$\frac{\partial P_1(t,z)}{\partial t} = b_1 \frac{\partial^2 P_1}{\partial z^2} - \beta_1 \frac{\varepsilon}{R_1} \frac{\partial}{\partial t} \int_0^{R_1} P_2(t,x_1,z) dx_1 - \beta_2 \frac{1-\varepsilon}{R_2} \frac{\partial}{\partial t} \int_0^{R_2} P_3(t,x_2,z) dx_2$$
(1)

with the initial condition:

$$P_1(t,z)|_{t=0} = P_E,$$
(2)

the boundary conditions (for variable z)

$$P_1(t,z)|_{z=0} = 0;$$
 $\frac{\partial P_1}{\partial z}|_{z=h} = 0$ (impermeability condition); (3)

2.2. Consolidation equations for particles

Problems B_{1,2}: to find the limited solutions of the consolidation equations for the nanoporous particles (radius R_i) in the domain $D_2 = \{(t, x_1, x_2, z) : t > 0, |x_1| < R_1, |x_2| < R_2, 0 < z < h\}$:

$$\frac{\partial P_i}{\partial t} = b_i \frac{\partial^2 P_i}{\partial x_j^2}, \ i = \overline{2,3}, \ j = \overline{1,2}$$
(4)

with the initial conditions:

$$P_i\Big|_{t=0} = P_E(z), \ i = 2,3 \tag{5}$$

the boundary conditions (for radial variable x_j) are :

$$\frac{\partial P_i}{\partial x_j}\Big|_{x_j=0} = 0; \qquad P_i(t, x_j, z)_{|x_j=R_j} = P_1(t, z).$$
(6)

2.3. Nomenclature

 P_1 - liquid pressure in interparticle space, P_2 , P_3 - liquid pressure in intraparticle space 1 and intraparticle space 2 (interior of spherical particles 1 and 2) in accordance, b_1 - is a consolidation coefficient in interparticle space, b_2 , b_3 - consolidation coefficients in intraparticle space 1 and intraparticle space 2, β_1 , β_2 - elasticity factor of the particles 1 and 2 in accordance, h - is layer thickness, R_1 , R_2 - radius of particles 1 and 2.

3. The analytical solution of the model

A pressure profiles in *interparticle spaces* and *intraparticle spaces* 1 and *intraparticle spaces* 2. The analytical solution of the problem is found using the operational Heaviside's method, Laplace integral and Fourier integral transformations.

Applying the finite integral Fourier transform (cos) [3, 4]:

$$F_{c}\left[P_{i}(t,x_{j},z)\right] = \int_{0}^{n_{j}} P_{i}(t,x_{j},z)\vartheta(x_{j},\eta_{m_{j}})dx_{j} = \int_{0}^{n_{j}} P_{i}(t,x_{j},z)\cos\eta_{m_{j}}x_{j}dx_{j} \equiv P_{im_{j}}(t,z), \ i = \begin{cases} 2, \quad j=1\\ 3, \quad j=2 \end{cases};$$

$$F_{c}^{-1}\left[P_{im_{j}}(t,z)\right] = \sum_{m_{j}=0}^{\infty} P_{im_{j}}(t,z)\frac{\vartheta(x_{j},\eta_{m_{j}})}{\left\|\vartheta(x_{j},\eta_{m_{j}})\right\|^{2}} = \frac{2}{R_{1}}\sum_{m_{i}=0}^{\infty} P_{im_{j}}(t,z)\cos\eta_{m_{j}}x_{j} \equiv P_{i}(t,x_{j},z), \ i = \begin{cases} 2, \quad j=1\\ 3, \quad j=2 \end{cases};$$

$$F_{c}\left[\frac{\partial P_{i}}{\partial x_{j}^{2}}\right] = \int_{0}^{R} \frac{\partial^{2} P_{i}}{\partial x_{j}^{2}}\vartheta(x_{j},\eta_{m_{j}})dx_{j} = -\eta_{m_{j}}^{2}P_{im_{j}}(t,z) + (-1)^{m_{j}}\eta_{m_{j}}P_{1}(t,z), \ i = \begin{cases} 2, \quad j=1\\ 3, \quad j=2 \end{cases};$$
were $\vartheta(x_{j},\eta_{m_{j}}) = \cos\eta_{m_{j}}x_{j}, \ \eta_{m_{j}} = \frac{2m_{j}+1}{2R_{i}}\pi, \ m_{j} = \overline{0,\infty} \ - \ \text{are the spectral functions and spectral}}$

numbers of integral Fourier transform (cos), we obtain the solutions of the problems B_1, B_2 :

$$P_{2}(t,x,z) = P_{E}(z)\frac{2}{R_{1}}\sum_{m_{1}=0}^{\infty}\frac{(-1)^{m_{1}}}{\eta_{m_{1}}}e^{-b_{2}\eta_{m_{1}}^{2}t}\cos\eta_{m_{1}}x + \frac{2}{R_{1}}\sum_{m_{1}=0}^{\infty}(-1)^{m_{1}}b_{2}\eta_{m_{1}}\int_{0}^{t}e^{-b_{2}\eta_{m_{1}}^{2}(t-\tau)}P_{1}(\tau,z)dz\cos\eta_{m_{1}}x, \ |x| \le R_{1}$$

$$P_{3}(t,x,z) = P_{E}(z)\frac{2}{R_{2}}\sum_{m_{2}=0}^{\infty}\frac{(-1)^{m_{2}}}{\eta_{m_{2}}}e^{-b_{3}\eta_{m_{2}}^{2}t}\cos\eta_{m_{2}}x + \frac{2}{R_{3}}\sum_{m_{2}=0}^{\infty}(-1)^{m_{2}}b_{3}\eta_{m_{2}}\int_{0}^{t}e^{-b_{3}\eta_{m_{2}}^{2}(t-\tau)}P_{1}(\tau,z)dz\cos\eta_{m_{2}}x, \ |x| \le R_{2}$$

$$(7)$$

Substituting the expressions (7) into the consolidation equation (1), after a series of transformations and successive application to the problem (1)-(3) of the integral Laplace transform [3] and the finite integral Fourier transform (sin):

$$F_{s}\left[P_{1}^{*}(s,z)\right] = \int_{0}^{h} P_{1}^{*}(s,z) \cdot V(z,\lambda_{n}) dz = \int_{0}^{h} P_{1}^{*}(s,z) \cdot \sin \lambda_{n} z dz = P_{1,n}^{*}(s),$$

$$F_{s}^{-1}\left[P_{1,n}^{*}(s)\right] = \sum_{n=0}^{\infty} P_{1,n}^{*}(s) \frac{V(z,\lambda_{n})}{\|V(z,\lambda_{n})\|^{2}} = \frac{2}{h} \sum_{n=0}^{\infty} P_{1,n}^{*}(s) \sin \lambda_{n} z \equiv P_{1}^{*}(s,z),$$

$$F_{s}\left[\frac{d^{2}P_{1}^{*}(s)}{dz^{2}}\right] = -\lambda_{n}^{2} P_{1,n}^{*}(s,z),$$

were $V(z,\lambda_n) = \sin \frac{2n+1}{2h}\pi$ – are the spectral functions and $\lambda_n = \frac{2n+1}{2h}\pi$ – are the spectral numbers of integral Fourier transformation (Sin-Fourier).

Applying the integral operator of the inverse integral Laplace transformation to expression (8) we obtain [5]:

$$\left(\lambda^{n} + \frac{s}{b_{1}} \left(1 + 2\frac{\beta_{1}\varepsilon}{R_{1}^{2}} \sum_{m_{1}=0}^{\infty} \frac{1}{s/b_{2} + \eta_{m_{1}}^{2}} + 2\frac{\beta_{2}\left(1 - \varepsilon\right)}{R_{2}^{2}} \sum_{m_{2}=0}^{\infty} \frac{1}{s/b_{3} + \eta_{m_{2}}^{2}}\right) \right) P_{1_{n}}^{*}(s) = \\ = -\frac{1}{b_{1}} \left(2\frac{\beta_{1}\varepsilon}{R_{1}^{2}} \sum_{m_{1}=0}^{\infty} \frac{s/b_{2}}{s/b_{2} + \eta_{m_{1}}^{2}} + 2\frac{\beta_{2}\left(1 - \varepsilon\right)}{R_{2}^{2}} \sum_{m_{2}=0}^{\infty} \frac{s/b_{3}}{s/b_{3} + \eta_{m_{2}}^{2}}\right) \frac{P_{E}}{\lambda_{n}} + \\ + \left(\frac{1 + \beta_{1}\varepsilon}{b_{1}} + \frac{1 + \beta_{2}(1 - \varepsilon)}{b_{1}}\right) P_{E} \frac{1}{\lambda_{n}}$$

Using seris [3, 5]

$$\sum_{m_1=0}^{\infty} \frac{1}{s/b_2 + \eta_{m_1}^2} = \frac{R_1}{2} \sqrt{\frac{b_2}{s}} th\left(\sqrt{\frac{s}{b_2}}R_1\right)$$
$$\sum_{m=0}^{\infty} \frac{s}{\eta_m^2\left(s + b_2\eta_m^2\right)} = \sum_{m=0}^{\infty} \left(\frac{1}{\eta_m^2} - \frac{1}{\frac{s}{b_2} + \eta_m^2}\right) = \frac{R_1^2}{2} - \frac{R_1}{2} \sqrt{\frac{b_2}{s}} th\left(\sqrt{\frac{s}{b_2}}R_1\right)$$

as result we obtain

$$P_{1_{n}}^{*}(s) = \left(b_{1}\lambda^{n} + s + \beta_{1}\varepsilon\frac{\sqrt{b_{2}}}{R_{1}}\sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_{2}}}R_{1}\right) + \beta_{2}\left(1-\varepsilon\right)\frac{\sqrt{b_{3}}}{R_{2}}\sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_{3}}}R_{2}\right)\right)^{-1} \cdot \left(2 + \frac{\beta_{1}\varepsilon}{R_{1}}\sqrt{\frac{b_{2}}{s}}th\left(\sqrt{\frac{s}{b_{2}}}R_{1}\right) + \frac{\beta_{2}\left(1-\varepsilon\right)}{R_{2}}\sqrt{\frac{b_{3}}{s}}th\left(\sqrt{\frac{s}{b_{3}}}R_{2}\right)\right)P_{E}\frac{1}{\lambda_{n}}$$

$$(8)$$

Introducing the notation

$$\phi(s,\lambda^n) = s + b_1\lambda^n + \beta_1\varepsilon \frac{\sqrt{b_2}}{R_1}\sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right) + \beta_2(1-\varepsilon)\frac{\sqrt{b_3}}{R_2}\sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)$$

and applying the integral operator of the inverse Laplace transformation, we obtain the formula for making the transition to the original in equation (8):

$$P_{1,n}(t) = P_E \frac{2}{\lambda_n} L^{-1} \left[\frac{1}{\phi\left(s,\lambda^n\right)} \right] + P_E \frac{\beta_1 \varepsilon}{\lambda_n} L^{-1} \left[\frac{1}{\phi\left(s,\lambda^n\right)} \right] * L^{-1} \left[\frac{sh\sqrt{\frac{s}{b_2}R_1}}{\sqrt{\frac{s}{b_2}R_1 ch\sqrt{\frac{s}{b_2}R_1}}} \right] + P_E \frac{\beta_2(1-\varepsilon)}{\lambda_n} L^{-1} \left[\frac{1}{\phi\left(s,\lambda^n\right)} \right] * L^{-1} \left[\frac{sh\sqrt{\frac{s}{b_3}R_2}}{\sqrt{\frac{s}{b_3}R_2 ch\sqrt{\frac{s}{b_3}R_2}}} \right]$$
(9)

where $L^{-1}[...]$ - integral operator of inverse L laplce transformation, " * " – is an operator of convolution of both functions.

Now we can consider the next equation:

$$s + b_1 \lambda^n + \beta_1 \varepsilon \frac{\sqrt{b_2}}{R_1} \sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_2}} R_1\right) + \beta_2 (1 - \varepsilon) \frac{\sqrt{b_3}}{R_2} \sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_3}} R_2\right) = 0$$

Replacing $i\sqrt{s} = v$ or $s = -v^2$, we obtain:

$$v^{2} - b_{1}\lambda_{n}^{2} - \beta_{1}\varepsilon v \frac{\sqrt{b_{2}}}{R_{1}} tg\left(\frac{vR_{1}}{\sqrt{b_{2}}}\right) - \beta_{2}(1-\varepsilon)v \frac{\sqrt{b_{3}}}{R_{2}} tg\left(\frac{vR_{2}}{\sqrt{b_{3}}}\right) = 0.$$

$$(10)$$

According to Heviside theorem one can obtain the expression of transfer to original [4]:

$$\cdot L^{-1} \left[\frac{1}{s + b_1 \lambda^n + \beta_1 \varepsilon \frac{\sqrt{b_2}}{R_1} \sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_2}} R_1\right) + \beta_2 (1 - \varepsilon) \frac{\sqrt{b_3}}{R_2} \sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_3}} R_2\right)} \right]^{-1} = \frac{1}{2\pi i} \int_{\gamma} \frac{e^{st} ds}{s + b_1 \lambda^n + \beta_1 \varepsilon \frac{\sqrt{b_2}}{R_1} \sqrt{s} th\left(\sqrt{\frac{s}{b_2}} R_1\right) + \beta_2 (1 - \varepsilon) \frac{\sqrt{b_3}}{R_2} \sqrt{s} th\left(\sqrt{\frac{s}{b_3}} R_2\right)}^{-1} = \frac{\varepsilon^{st}}{\frac{d}{ds} \left[s + b_1 \lambda^n + \beta_1 \varepsilon \frac{\sqrt{b_2}}{R_1} \sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_2}} R_1\right) + \beta_2 (1 - \varepsilon) \frac{\sqrt{b_3}}{R_2} \sqrt{s} \cdot th\left(\sqrt{\frac{s}{b_3}} R_2\right)} \right]_{s = -v_{jn}^2} ,$$

$$(11)$$

where v_{jn} , $j = \overline{1,\infty}$; $n = \overline{0,\infty}$ – the roots of transcendental equation (10). Calculating of the denominator in (11):

$$\frac{d}{ds}\left[s+b_{1}\lambda^{n}+\beta_{1}\varepsilon\frac{\sqrt{b_{2}}}{R_{1}}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_{2}}}R_{1}\right)+\beta_{2}(1-\varepsilon)\frac{\sqrt{b_{3}}}{R_{2}}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_{3}}}R_{2}\right)\right]_{s=-v_{jn}^{2}}$$

$$=1+\beta_{1}\varepsilon\frac{\sqrt{b_{2}}}{2R_{1}}\left[\frac{1}{v_{jn}}tg\left(v_{jn}\frac{R_{1}}{\sqrt{b_{2}}}\right)+\frac{R_{1}}{\sqrt{b_{2}}}\frac{1}{\cos^{2}\left(v_{jn}\frac{R}{\sqrt{b_{2}}}\right)}\right]+\beta_{2}(1-\varepsilon)\frac{\sqrt{b_{3}}}{2R_{2}}\left[\frac{1}{v_{jn}}tg\left(v_{jn}\frac{R_{2}}{\sqrt{b_{3}}}\right)+\frac{R_{2}}{\sqrt{b_{3}}}\frac{1}{\cos^{2}\left(v_{jn}\frac{R_{2}}{\sqrt{b_{3}}}\right)}\right]$$

Then, as result, the expression (11) will have the vie:

$$L^{-1}\left[\frac{1}{s+b_1\lambda^n+\beta_1\varepsilon\frac{\sqrt{b_2}}{R_1}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_2}}R_1\right)+\beta_2\left(1-\varepsilon\right)\frac{\sqrt{b_3}}{R_2}\sqrt{s}\cdot th\left(\sqrt{\frac{s}{b_3}}R_2\right)}\right]=\sum_{j=1}^{\infty}\frac{e^{-\nu_{jn}^2t}}{1+\Phi\left(\nu_{jn}\right)}\cdot$$

were

$$\Phi(v_{jn}) = 1 + \beta_{1} \varepsilon \frac{\sqrt{b_{2}}}{2R_{1}} \left(\frac{1}{v_{jn}} tg\left(v_{jn}\frac{R_{1}}{\sqrt{b_{2}}}\right) + \frac{R_{1}}{\sqrt{b_{2}}} \frac{1}{\cos^{2}\left(v_{jn}\frac{R}{\sqrt{b_{2}}}\right)} \right) + \beta_{2}(1-\varepsilon)\frac{\sqrt{b_{3}}}{2R_{2}} \left(\frac{1}{v_{jn}} tg\left(v_{jn}\frac{R_{2}}{\sqrt{b_{3}}}\right) + \frac{R_{2}}{\sqrt{b_{3}}} \frac{1}{\cos^{2}\left(v_{jn}\frac{R_{2}}{\sqrt{b_{3}}}\right)} \right)$$

$$L^{-1} \left[\frac{sh\sqrt{\frac{s}{b_2}}R_1}{\sqrt{\frac{s}{b_2}}R_1 \cdot ch\sqrt{\frac{s}{b_2}}R_1} \right] = \sum_{k=0}^{\infty} \frac{i(-1)^k e^{-b_2 \eta_k^2 t}}{\frac{d}{ds} \left[\sqrt{\frac{s}{b_2}}R_1 \cdot ch\sqrt{\frac{s}{b_2}}R_1 \right]_{s=-\eta_k^2}} = -b_2 \frac{2}{R_1^2} \sum_{k=0}^{\infty} e^{-b_2 \eta_k^2 t} \cdot L^{-1} \left[\frac{sh\sqrt{\frac{s}{b_3}}R_2}{\sqrt{\frac{s}{b_3}}R_2} \right] = \sum_{k=0}^{\infty} \frac{i(-1)^k e^{-b_3 \eta_k^2 t}}{\frac{d}{ds} \left[\sqrt{\frac{s}{b_3}}R_2 ch\sqrt{\frac{s}{b_3}}R_2 \right]_{s=-\eta_k^2}} = -b_3 \frac{2}{R_2^2} \sum_{k=0}^{\infty} e^{-b_2 \mu_k^2 t}$$
(12)

In result of this transforms, we obtain the original of function P_1

$$P_{1}(t,z) = P_{E} \frac{2}{h} \sum_{n=0}^{\infty} \sum_{j=1}^{\infty} \frac{e^{-\nu_{jn}^{2}t}}{\Phi(\nu_{jn})} \left[1 - \beta_{1} \varepsilon \frac{2}{R_{1}^{2}} \sum_{k=0}^{\infty} \frac{\left(\eta_{k}^{2} - \frac{\nu_{jn}^{2}}{b_{2}}\right)}{-\beta_{2}(1-\varepsilon) \frac{2}{R_{2}^{2}} \sum_{k=0}^{\infty} \frac{1-e}{\left(\mu_{k}^{2} - \frac{\nu_{jn}^{2}}{b_{3}}\right)t}}{\left(\mu_{k}^{2} - \frac{\nu_{jn}^{2}}{b_{3}}\right)} \right] \frac{\sin \lambda_{n} z}{\lambda_{n}}, \quad (13)$$

which describe the pressure distributions in the *interparticle space*.

Here v_{jn} , $j = \overline{1,\infty}$; $n = \overline{0,\infty}$ – the roots of transcendental equation (10).

$$\eta_k = \frac{(2k+1)\pi}{2R_1}, \ k = \overline{0,\infty}$$
 - are the roots of equation $ch\left(\sqrt{\frac{s}{b_2}}R_1\right) = 0, \ (s=i\eta, \ i-\text{ imaginary unit}),$

$$\mu_k = \frac{(2k+1)\pi}{2R_2}, \ k = \overline{0,\infty}$$
 – are the roots of equation $ch\left(\sqrt{\frac{s}{b_3}}R_2\right) = 0, \ (s=i\mu)$

$$\lambda_n = \frac{2n+1}{2h}\pi$$
 – are the spectral numbers of integral Fourier transformation (Sin-Fourier).

Substituting into formulas (7) the analytical expression of pressure distributions in the *interparticle* space $P_1(t,z)$, calculated according to (13), we obtain the final expressions for determining the time-space distributions of pressures $P_2(t,x,z)$ and $P_3(t,x,z)$ in the spaces of nanoporous particles: *intraparticle spase* 2 and *intraparticle spase* 3 in accordance.

4. Numerical modelisation and discussion.

As a part of the simulation stage, a special software complex was developed to study the internal kinetics processes of filtration in multidimensional nanoporous particle media. Such software was built with a modern approach to software design and keeping in mind software engineering best practices.

The main goal is to allow the quick study of filtration processes for scientists and staff by reducing the time from inputting parameters of nanoporous media to the graphical visualization of key performance metrics of the filtration process.

Results of the filtration kinetics process study are presented below. The process parameters used for simulations are: h=0.01m, R₁=0.008 m, R₂=0.004 m, $b_1 = 10^{-7}$ m²/s, $b_2 = 2 \ 10^{-7}$ m²/s, $b_3 = 10^{-8}$ m²/s, $\beta_1 = 0.1$, $\beta_2 = 0.15$, $\varepsilon = 0.5$. The media consists of two types of multidimensional nanoporous particles of different kinetic properties.

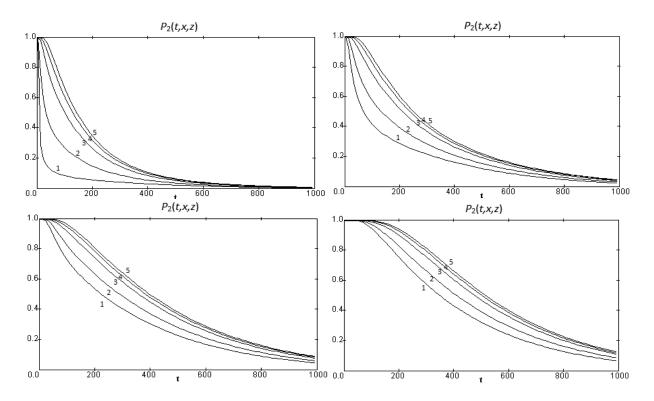


Figure 2: Distribution of dimensionless pressure in the intraparticles space1 $P_2(t,x,z)$ versus time t, [s] in different sections of dimensionless layer: a) Z=0.05; b) Z=0.25; c) Z=0.5; d) Z=1 (Z=z/h); 1 - X=1.0 2 - X=0.8; 3 - X=0.6; 4 - X=0.4; 5 - X=0.05 (X=x_1/R_1)

Figure 2 shows the dimensionless liquid pressure profiles inside the porous particles of first type $P_2(t,x,z)$ in time t[s]. The temporal pressure profiles were simulated for different layer sections: Z=1 (top of layer), Z=0.5 and Z=0.25 (a middle sections of layer), and Z=0 (surface of the filter medium. In the proposed images are clear to observe that liquid pressure is higher in the center of particles (X=0.05) and decline in direction of liquid expulsion on a particles surface X=1 ($x_m = R_m$). At the particles edge the pressure in micropores tends to the pressure in macropores $P_1(t,z)$. Also, it is worth to note, that liquid pressure declines rapidly on the particles surface (X=1) than in the middle sections (0.4, 0.6, 0.8) or particles center (X=0.05).

The difference between the temporal pressure profiles becomes more significant for particles located on top of the later (Z=0). However, even in sections close to the central axe of particles (X=0), the liquid pressure drops rather rapidly.

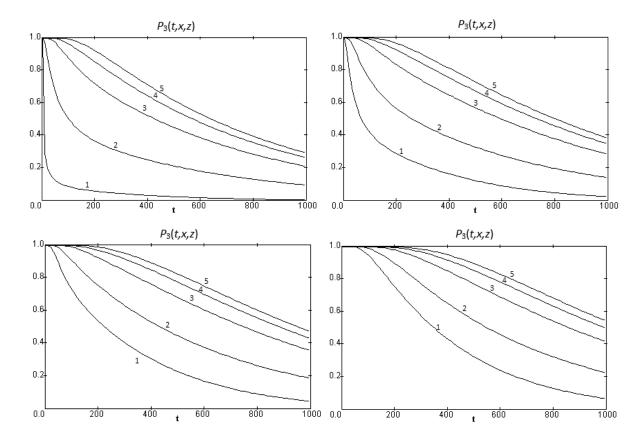


Figure 3. Distribution of dimensionless pressure in the intraparticles space $P_3(t,x,z)$ versus time t, [s] in different sections of dimensionless layer: a) Z=0.05; b) Z=0.25; c) Z=0.5; d) Z=1 (Z=z/h); $1 - X=1.0 \ 2 - X=0.8; \ 3 - X=0.6; \ 4 - X=0.4; \ 5 - X=0.05 \ (X=x_2/R_2)$

Figure 3 shows the temporal profiles of dimensionless liquid pressure inside of porous particles of second type (small) in time t[s]. Same as before, the temporal pressure profiles were simulated for four different sections of media layer: Z=1, 0.25, 0.5 and 0.05. The consolidation coefficient for these types of particles characterizes less destroyed cellular tissue compared to the particles of the first type. Like in a previous example, the presented profiles show liquid pressure drops on the surface of particles (X=1) are more rapid than for sections close to the particle's center (X=0.05), and overall decline is more significant when Z leads to 0. However, appreciable retardation of liquid pressure drop can be detected in micropores of particles.

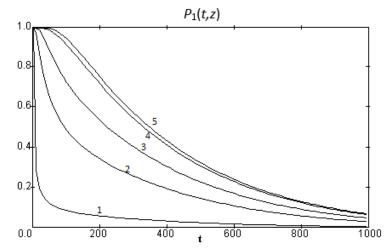


Figure 4. Distribution of dimensionless pressure in the interparticles space $P_1(t,z)$: 1 - Z = 0.05, 2 - Z = 0.3, 3 - Z = 0.5, 4 - Z = 0.7; 5 - Z=1.0 (Z=z/h)

Figure 4 shows distributions of pressure profiles in interparticles space $P_1(t,z)$ at different sections of nanoporous media.

5. Conclusions

During this research, was developed a foundation of scientific information technologies for nanoporous filtration systems with multidimensional nanoporous particles. A phenomenological model of the solid-liquid expression of a liquid containing various-sized nanoporous moisturecontaining particles as a multi-level porous system with interparticle and intraparticle networks for liquid flows is formulated.

The filtration-consolidation equations were formulated for both intrerparticle and two intraparticle networks considering the pressure profiles. It was assumed, that for nanoporous media, the interparticle network forms the first porosity with a low storage capacity, while the intraparticle network forms two-second porosities with a high storage capacity. High-speed analytical solutions describe the spatiotemporal pressure distributions in the interparticle space, intraparticle space (particles of radius R1), and intraparticle space (particles of radius R2, R1>R2) are obtained for real nanoporous geomedia with two high characteristics of stability and permeability. Numerical simulation results showed a joint pressure drop in the intraparticle network and an increase in the consolidation kinetics for the two types of differently sized nanoporous particles.

In the framework of scientific information technologies, specialized software has been created for the study of nanoporous filtration systems in media with multidimensional nanoporous particles based on the described mathematical model. The main goals pursued in software design were to allow the quick and detailed study of filtration processes in nanoporous for scientists, the ability to run on any modern platforms, high-performance numerical modeling, and friendly UI/UX. The use of software engineering best practices made it possible to create a software design that could easily be expanded or evolved by adding new classes of scientific and special services, as well as future improvements, to meet new requirements.

6. References

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